Bounding the set of quantum correlations

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We introduce a hierarchy of conditions necessarily satisfied by any distribution $P_{\alpha\beta}$ representing the probabilities for two separate observers to obtain outcomes α and β when making local measurements on a shared quantum state. Each condition in this hierarchy is formulated as a semidefinite program. Our approach can be used to obtain upper-bounds on the quantum violation of an arbitrary Bell inequality. It yields, for instance, tight bounds for the violations of the Collins et al. inequalities.

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The correlations between two separated physical systems can be characterized by the joint probabilities $P_{\alpha\beta}$ that an observer who performs a measurement X on the first system gets an outcome $\alpha \in X$ and that an observer making a measurement Y on the second system gets an outcome $\beta \in Y$. If the observed system is in an entangled state, these joint probabilities may violate a Bell inequality, implying that quantum theory is not, in Bell's terminology, locally causal [1]. Although quantum correlations are not constrained by Bell's locality principle, they are not arbitrary since a general joint distribution $P_{\alpha\beta}$ cannot always be viewed as originating from measurements performed on a shared quantum system [2].

In this paper, we investigate the restrictions on bipartite correlations imposed by the quantum formalism. The question that we seek to answer is the following: Given an arbitrary distribution $P_{\alpha\beta}$, do there exist a quantum state ρ on a joint Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ and local measurement operators $E_\alpha = \tilde{E}_\alpha \otimes I$ and $E_\beta = I \otimes \tilde{E}_\beta$, such that $P_{\alpha\beta} = \mathrm{tr}\,(E_\alpha E_\beta\, \rho)$?

From a fundamental point of view, one motivation for studying this problem is simply to understand which correlations can arise between two systems within our current description of nature. Another is to develop tools to detect the possible non-quantumness of some set of empirically observed correlations. Practically, answering the above question is of interest for various applications in quantum science, for instance, for the design of nonlocality tests more resistant to imperfections. In general, characterizing the set of quantum correlations is essential to understand better the extent to which quantum mechanics is useful in information processing tasks such as communication complexity and key distribution. An usual problem in these contexts is to determine what is the maximal violation of a Bell inequality allowed by quantum mechanics.

Answering the above question is in general a difficult task; the simple strategy of searching over all quantum states ρ and measurement operators E_μ, which in principle can be of arbitrary dimension, is clearly unfeasible. The first to address the problem of characterizing the set of quantum correlations was Tsirelson [3]. Tsirelson introduced a useful representation of quantum correlations in the special case that measurements have binary outcomes and that one considers correlation functions of the form $C_{XY} = \sum_{\alpha\in X}\sum_{\beta\in Y} \alpha\beta\, P_{\alpha\beta}$ rather than the full set of probabilities $P_{\alpha\beta}$. He derived in particular the maximal quantum violation for the Clauser-Horne-Shimony-Holt (CHSH) inequality [4]. There are few results that extend significantly Tsirelsons's analysis to other situations, although there have been several rederivations of his findings and attempts to generalize them [5]. Among those, we mention in particular the works of Landau [6] and Wehner [7], who realized that deciding if a set of correlations admits a quantum representation, in the specific case considered by Tsirelson, can be cast as a semidefinite program (SDP), a particular convex optimization problem for which powerful computational and theoretical methods have been developed [8].

Our approach is similar in spirit to the one of Landau and Wehner, but it applies to arbitrary situations. We introduce here a family of conditions necessarily satisfied by any distribution of quantum probabilities. Verifying that any one of these conditions is satisfied amounts to solve a SDP. Seen as a whole, our family of conditions exhibits a hierarchical structure, in the sense that it corresponds to a sequence of conditions, each condition in the sequence being stronger than the preceding one. We present two applications of our approach. First, we derive a non-linear inequality satisfied by quantum mechanics which strengthens a previous inequality due to Tsirelson [9], Landau [6] and Masanes [10]. As a second application, we give a tight bound for the violations of the Collins et al. inequalities [11].

Preliminaries. Before entering in the details of our construction, let us first give some definitions and precise the assumptions made through this paper. We assume that the two parties, Alice and Bob, choose their measurements from a finite set of possibilities, and that each measurements may yield one out of a finite set of outcomes. Note that we think of outcomes corresponding to different measurements as being labeled distinctly, so that each outcome α of Alice (or β of Bob) is unambiguously associated to a unique measurement X (or Y).

Refining the statement made earlier, we say that a distribution $P_{\alpha\beta}$ admits a quantum representation if there exist a joint quantum state ρ on $\mathcal{H}_A \otimes \mathcal{H}_B$, a set of *projection* operators $E_\alpha = \tilde{E}_\alpha \otimes I$ acting on Alice's system and a set of *projection* operators $E_\beta = I \otimes \tilde{E}_\beta$ acting on Bob's system, such that

$$P_{\alpha\beta} = \mathrm{tr}\,(E_\alpha E_\beta\,\rho)\;. \tag{1}$$

Projectors corresponding to outcomes belonging to the same measurement M should (i) be orthogonal: $E_\mu E_\nu = 0$ for $\mu,\nu \in M$, $\mu \neq \nu$, and (ii) sum to the identity: $\sum_{\mu\in M} E_\mu = I$. By definition, we also have that (iii) $E_\mu^2 = E_\mu^\dagger = E_\mu$ and that (iv) the projectors on Alice's and Bob's side commute with each other: $[E_\alpha, E_\beta] = 0$.

Note that the most general description of a quantum measurement corresponds to a positive operator valued measure (POVM) rather than a set of projection operators. But since a POVM can be viewed as a projective measurement on a system of larger dimension, and since we do not impose any constraints on the dimension of the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, no generality is lost with our definition.

Necessary conditions for quantum probabilities. We now introduce a family of conditions satisfied by any quantum distribution $P_{\alpha\beta}$. We thus start by assuming that there exist a quantum state ρ and a set $\{E_\mu\}$ of projection operators satisfying Eq. (1) and the properties (i)-(iv), and seek new implications from these assumptions.

By taking products of the operators E_μ and linear combinations of such products, we can define new operators, for instance $E_\alpha E_\beta E_{\alpha'}$ or $\sum_\alpha c_\alpha E_\alpha$ (note that these new operators are not necessarily projection operators anymore, nor even hermitian operators). Let $\mathcal{S} = \{S_1, \ldots, S_n\}$ be a set of n such operators. Associate to the set $\mathcal{S}$ a $n \times n$ matrix Γ through

$$\Gamma_{ij} = \mathrm{tr}\left(S_i^\dagger S_j\,\rho\right)\;. \tag{2}$$

By construction, the matrix Γ is hermitian, it satisfies the linear identities

$$\sum_{i,j} c_{ij}\Gamma_{ij} = 0 \qquad \text{if } \sum_{i,j} c_{ij} S_i^\dagger S_j = 0\,, \tag{3}$$

$$\begin{aligned}\sum_{i,j} c_{ij}\Gamma_{ij} &= \sum_{\alpha,\beta} d_{\alpha\beta} P_{\alpha\beta}\\ &\qquad \text{if } \sum_{i,j} c_{ij} S_i^\dagger S_j = \sum_{\alpha,\beta} d_{\alpha\beta} E_\alpha E_\beta\,,\end{aligned} \tag{4}$$

and it is positive semidefinite,

$$\Gamma \succeq 0\,. \tag{5}$$

The linear constraints (3) directly follow from the linearity of the trace in (2). The important point is that they partly reflect the properties *(i)-(iv)* satisfied by the operators E_μ. For instance suppose that $\mathcal{S}$ contains an operator $S_j = E_\mu$ and a subset of operators $\{S_k \mid k \in \mathcal{K}\} = \{E_\mu E_\nu \mid \nu \in M\}$ for some measurement M. Then, property (ii) implies $\sum_{k\in\mathcal{K}} S_k = \sum_{\nu\in M} E_\mu E_\nu = E_\mu = S_j$ and thus $\sum_{k\in\mathcal{K}} \Gamma_{ik} = \Gamma_{ij}$. As another example, suppose that $S_i = E_\alpha$ and $S_j = E_\beta E_{\alpha'}$ with $\alpha, \alpha' \in X$ and $\alpha \neq \alpha'$. Then, using successively properties (iii), (iv) and (i), we find $S_i^\dagger S_j = E_\alpha E_\beta E_{\alpha'} = E_\alpha E_{\alpha'} E_\beta = 0$, and thus $\Gamma_{ij} = 0$. The conditions (4) are obtained by making use of (1) in (2) and relate the entries of the matrix Γ to the specific set of probabilities $P_{\alpha\beta}$ under consideration. Finally, to establish (5), remember that an $n \times n$ matrix Γ is semidefinite positive if and only if $v^\dagger \Gamma v \geq 0$ for all $v \in \mathbb{C}^n$. Expanding this expression, we get

$$\begin{aligned} v^\dagger \Gamma v &= \sum_{i,j} v_i^* \mathrm{tr}\left(S_i^\dagger S_j \rho\right) v_j \\ &= \mathrm{tr}\Big[\big(\sum_i v_i S_i\big)^\dagger \big(\sum_j v_j S_j\big)\,\rho\Big] \geq 0\,,\end{aligned} \tag{6}$$

since ρ is a positive operator.

For any a quantum distribution $P_{\alpha\beta}$, there thus necessarily exist for each set $\mathcal{S}$ a matrix Γ satisfying the linear constraints (3) and (4) and the condition of positivity (5). Conversely, if for some $\mathcal{S}$ it is not possible to find a matrix Γ satisfying these properties, then we can conclude that the correlations characterized by the distribution $P_{\alpha\beta}$ cannot be reproduced through local measurements on a quantum state. Determining if there exists a positive semidefinite matrix satisfying a set of linear constraints is a typical instance of semidefinite programming [8]. All the techniques developed in this context can thus be applied to evaluate our conditions.

To give a concrete example of our method, consider the case where $\mathcal{S} = \{E_\alpha\} \cup \{E_\beta\}$ is simply the set of all projectors of Alice and of Bob. Suppose that they are m different measurement outcomes $\alpha = 1, \ldots, m$ for Alice and m different outcomes $\beta = m+1, \ldots, 2m$ for Bob. Then $\mathcal{S} = \{E_1, \ldots, E_m, E_{m+1}, \ldots, E_{2m}\}$ and applying the above construction, we find that Γ is a $2m \times 2m$ matrix of the form

$$\Gamma = \begin{pmatrix} Q & P \\ P^T & R \end{pmatrix}\,, \tag{7}$$

where the submatrix P is simply the $m \times m$ table of probabilities with entries $P_{\alpha\beta}$, and the submatrices Q and R satisfy

$$\begin{aligned} Q_{\alpha\alpha} &= P_\alpha, \qquad Q_{\alpha\alpha'} = 0 \quad (\alpha, \alpha' \in X \text{ and } \alpha \neq \alpha')\,,\\ R_{\beta\beta} &= P_\beta, \qquad R_{\beta\beta'} = 0 \quad (\beta, \beta' \in Y \text{ and } \beta \neq \beta')\,,\end{aligned}$$

where $P_\alpha = \sum_{\beta\in Y} P_{\alpha\beta}$ and $P_\beta = \sum_{\alpha\in X} P_{\alpha\beta}$ are the marginal probabilities for Alice and Bob, respectively. The form of the matrix (7) is defined by the linear constraints (3) and (4). The only entries of Γ which are not determined by these constraints are the entries $Q_{\alpha\alpha'}$ with $\alpha \in X$ and $\alpha' \in X'$ belonging to different measurements of Alice ($X \neq X'$), and the entries $R_{\beta\beta'}$ with

$\beta \in Y$ and $\beta' \in Y'$ belonging to different measurements of Bob ($Y \neq Y'$). If the correlations $P_{\alpha\beta}$ are quantum, we know, however, that values can be assigned to these undetermined entries such that the overall matrix (7) is positive semidefinite, in accordance with (5). As we said above, semidefinite programming can be used to determine if the matrix (7) can be completed in such a way.

A hierarchy of conditions. We have shown how to design tests that distinguish correlations that can be reproduced through local measurements on a quantum state from those which cannot. Not all conditions build in this way are independent. It is easily established (see [12] for details) that if every operator in a set $\mathcal{S}$ can be written as a linear combination of operators in another set $\mathcal{S}'$, then the conditions obtained from $\mathcal{S}'$ are at least as constraining as the one obtained from $\mathcal{S}$, in the sense that if it is possible to complete the matrix Γ' associated to $\mathcal{S}'$, then it is also possible to complete the matrix Γ associated to $\mathcal{S}$.

From the set $\mathcal{T}_m = \{E_{\mu_1} \dots E_{\mu_m}\}$ of all products of m projectors, it is possible to construct all the operators that are linear combinations of products of m' projectors, with $m' \leq m$. A systematic way to check all our conditions thus consists in successively testing the conditions associated to the sets $\mathcal{T}_1 = \{E_\mu\}$, $\mathcal{T}_2 = \{E_\mu E_\nu\}$, etc., until a test possibly fails. Note that the condition based on the matrix (7) corresponds to the first test in this infinite hierarchy.

As an illustration, we now present three applications of our method.

Application 1. We start by reproducing a result due to Landau [6] and, in a slightly different context, to Wehner [7]. This example involves two measurements $X = 1, 2$ for Alice and two measurements $Y = 3, 4$ for Bob, where each measurement may yield one out of two outcomes, $+1$ or -1. This situation is thus characterized by sixteen probabilities $P_{(\pm X)(\pm Y)}$, to which we can associate eight projectors $E_{\pm M}$ ($M = 1, \dots, 4$). Suppose that we are interested not in the full probability distribution, but only in how much the outputs of Alice and Bob are correlated, that is, we are interested in the quantities $C_{XY} = \sum_{a,b} ab\, P_{(aX)(bY)}$ representing the probability that Alice's and Bob's outputs are equal, minus the probability that they are different. In quantum mechanics, we would write that $C_{XY} = \mathrm{tr}(\sigma_X^\dagger \sigma_Y\, \rho)$, with $\sigma_M = E_{+M} - E_{-M}$. Upon comparison with the definition (2), this suggests to build the condition based on the set $\mathcal{S} = \{\sigma_1, \dots, \sigma_4\}$. Taking into account the constraints (3) and (4), the corresponding 4×4 matrix Γ reads

$$\Gamma = \begin{pmatrix} 1 & u & C_{13} & C_{14} \\ & 1 & C_{23} & C_{24} \\ & & 1 & v \\ & & & 1 \end{pmatrix}, \tag{8}$$

where we have only given its upper triangular part since it is hermitian. The parameters u, v correspond to entries that are not determined by our construction; but if the correlation functions C_{XY} represent quantum correlations, it is possible to find values for u and v such that the matrix (8) is semidefinite positive. This is the criterion introduced by Landau [6]. From the characterization of quantum correlations given by Tsirelson [3] it follows that this condition is not only necessary but also sufficient for a set of correlations C_{XY} to admit a quantum representation, as noted also by Wehner [7]. That is, the correlation functions C_{XY} admit a quantum representation if and only if there exist values u and v such that (8) is semidefinite positive. The property of our condition to be sufficient in this specific case remains true for the generalizations of (8) to more measurement choices.

The criterion that we just introduced can be resolved analytically: there are values u and v such that (8) is semidefinite positive if and only if the correlations C_{XY} satisfy the inequality

$$|\mathrm{asin}\, C_{13} + \mathrm{asin}\, C_{14} + \mathrm{asin}\, C_{23} - \mathrm{asin}\, C_{24}| \leq \pi\,, \tag{9}$$

and the three other ones obtained by permutation of the measurements [6, 12]. These inequalities, which characterize the set of quantum correlations C_{XY}, were derived from a different perspective by Tsirelson [9] and Masanes [10].

Application 2. Consider the same example as above, but suppose that we are now interested in the full probability distribution. This is equivalent to say that in addition to the joint correlations C_{XY}, we are also interested in the marginal quantities $C_X = \sum_a a\, P_{aX}$ and $C_Y = \sum_b b\, P_{bY}$. A condition stronger than the preceding one is then obtained if we consider the set $\mathcal{S} = \{I, \sigma_1, \dots, \sigma_4\}$. The set $\mathcal{S}$ is in fact linearly equivalent to the set $\mathcal{T}_1 = \{E_{\pm 1}, \dots, E_{\pm 4}\}$ of all projectors and thus the resulting condition corresponds to the first test in the hierarchy defined earlier. The associated 5×5 matrix is

$$\Gamma = \begin{pmatrix} 1 & C_1 & C_2 & C_3 & C_4 \\ & 1 & u & C_{13} & C_{14} \\ & & 1 & C_{23} & C_{24} \\ & & & 1 & v \\ & & & & 1 \end{pmatrix}, \tag{10}$$

where as before u and v are undetermined quantities, which can be chosen so that $\Gamma \succeq 0$ if the correlations have a quantum representation. As above, this last condition can be evaluated analytically and leads to the following inequality

$$|\mathrm{asin}\, D_{13} + \mathrm{asin}\, D_{14} + \mathrm{asin}\, D_{23} - \mathrm{asin}\, D_{24}| \leq \pi \tag{11}$$

where

$$D_{ij} = \frac{C_{ij} - C_i C_j}{\sqrt{(1 - C_i^2)(1 - C_j^2)}}\,, \tag{12}$$

and to the inequalities obtained from (11) by permutation of the measurement choices. If we neglect the marginals by imposing $C_M = 0$ we recover the previous inequality (9). As a test on the full distribution, however, our inequality is more restrictive than (9) since it is easily verified that there are probability distributions that satisfy (9) but which violate (11). Note that (11) is not a sufficient condition for a full probability distribution to admit a quantum representation, as we have examples of correlations that satisfy (11) but which fail the successive step in the hierarchy.

Application 3. By maximizing the violation of a Bell inequality over the set of probability distributions satisfying one of our conditions, we obtain an upper-bound on the violation of this inequality by quantum mechanics (since such conditions are satisfied by every quantum distributions). A Bell inequality is a linear combination of the probabilities $P_{\alpha\beta}$, and since these probabilities are related in a linear way to the entries of the matrices Γ, obtaining such an upper-bound can be cast as a SDP. Consider for instance the CHSH expression, which in the notation of Application 1 reads $C_{13} + C_{14} + C_{23} - C_{24}$. Maximizing this expression over all distribution satisfying the criterion of Application 1 corresponds to the SDP

$$\begin{aligned} &\text{maximize} \quad C_{13} + C_{14} + C_{23} - C_{24} \\ &\text{subject to} \quad \begin{pmatrix} 1 & u & C_{13} & C_{14} \\ & 1 & C_{23} & C_{24} \\ & & 1 & v \\ & & & 1 \end{pmatrix} \succeq 0\,. \end{aligned} \tag{13}$$

The solution to this optimization problem is $2\sqrt{2}$, as noted by Wehner [7], and we thus recover the well-known Tsirelson bound. More generally, for any given Bell inequality, SDP's can be associated to each of the conditions $\mathcal{T}_1, \mathcal{T}_2, \ldots$ of our hierarchy, the solutions of which would yield a sequence $I_1 \geq I_2 \geq ...$ of upper-bounds on the quantum violation of the inequality. Note that after a finite number of such iterations, a tight bound may already be reached as the CHSH example and the following one show.

We have applied the approach just outlined to the Collins et al. inequalities [11]. This family of inequalities involves two measurement choices per party and d outputs per measurement, and can be viewed as a generalization of the CHSH inequality for systems of dimension greater than two. In [13], lower-bounds for the violation of the Collins et al. inequalities were given for $d = 3, \ldots, 8$ by exhibiting a particular set of measurements and a quantum state of dimension $d \times d$ yielding high violations of the inequalities. The quantum states had the particularity to be non-maximally entangled. For $d = 3$, the reported violation was $I_* = 2.9149$, the local bound of the inequality being $I_{\text{loc}} \leq 2$. We have numerically solved the SDP corresponding to the first tests in our hierarchy. For $d = 3$, the condition $\mathcal{T}_1$ yields the bound $I \leq 3.1547$, which is about 10% higher than the violation reported in [13]. The second condition $\mathcal{T}_2$, however, yields the bound $I \leq I_* = 2.9149$, proving that the partially entangled state and the measurements described in [13] are the optimal ones. We have also solved the SDP for $d = 4, \ldots, 8$. As for the $d = 3$ case, the first tests in the hierarchy are about 10% above the values presented in [13], but the second tests give the same results as the ones reported in [13], demonstrating that these are the optimal quantum violations.

Conclusion. The approach outlined in this paper opens a new way to study the correlations between two separate quantum systems. There are several possible extensions of our technique, for instance to systems of more than two parties, and many potential applications of it, among others to study non-local properties of quantum correlations, such as their monogamous character. A question that remains open is whether the hierarchy of conditions that we have introduced is complete, in the sense that a set of correlations satisfies every condition in the hierarchy if and only if it admits a quantum representation. We will address some of these questions, and present in more detail the results reported in this article, in a future paper [12].

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